

Final

**FOCUS REPORT**  
**New Chemicals Program**

**PART I: BACKGROUND**

Written By: KMB

FOCUS DATE: 8/6/2007

FOCUS CHAIR: M.WigLewis

COMPANY: Cognis Oleochemicals LLC

CASE NUMBER(S): P07-0563 through P07-0564 and

**PART II: SAT RESULTS**

HEALTH: 1-2 ECOTOX: 3 OCCUPATIONAL EXPOSURE: 1A CONSUMER EXPOSURE: 2 ENVIRONMENTAL RELEASES: 2

Additional SAT  
Information:

**PART III: OTHER FACTORS**

a. PRODUCTION VOLUME: [REDACTED] kg/yr

b. PROD VOL OTHER:

c. USE: Emulsifier for oil-mud drilling fluids

d. REGULATORY HISTORY: NRC

e. TEST DATA:

f. IMPORTED ☒ MANUFACTURED ☐ BOTH ☐

g. MSDS: ☒

h. CATEGORY: Aliphatic Amines CATEGORY 2:



2007-08-11 1:27

**PART IV: SUMMARY OF SAT ASSESSMENT**

CASE NUMBER: P07-0563/0564

FATE: Estimations for low weight. [REDACTED]

MW = [REDACTED]

Solid

log Kow = 2.90(E);

S = Disp./1.64 mg/L at 25 C (ICB/E)

VP < 1.0E-6 torr at 25 C (E)

BP > 400 C (E)

H [REDACTED]

log Koc = 7.63(E)

log Fish BCF = 1.54(E)

POTW removal (%) = 50-90 via sorption and possible partial biodeg

Time for complete ultimate aerobic biodeg = mo

Sorption to soils/sediments = strong

PBT Potential: P1B1T1

HEALTH: Not absorbed from the skin as the neat material, poor absorption from the skin if in solution (pchem), poor absorption from the GI tract and moderate absorption from the lung (analog). Concern for surfactant effects on the lung; irritation to eye, skin (chronic), mucous membranes and lung based on surfactant properties of the compounds. Also concern for possible lung toxicity from cationic binding to lung membranes.

☐ Test data: rat oral LD0 = 2000 mg/kg

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:  
fish 96-h LC50 < 1.0 P pH7 TOC<2

daphnid 48-h LC50 < 1.0 P pH7 TOC<2  
daphnid 48-h LC50 > 1000.0 M S,M pH? TOC94  
marine copepod 48-h LC50 > 10,000.0 M S,N pH? TOC?  
amphipod 10-d LC50 > 13,600.0 M S,N pH? TOC?  
green algal 96-h EC50 < 1.0 P pH7 TOC<2  
algal (Skele) 72-h EC50 r = 185.0 M S,N pH7 TOC?  
fish chronic value < 0.100 P pH7 TOC<2  
daphnid ChV < 0.100 P pH7 TOC<2  
algal ChV < 0.300 P pH7 TOC<2

Predictions are based on SAR-nearest analog analysis for aliphatic amines-fatty

; SAR chemical class = aliphatic amine-

; solid with mp unknown (P); S = dispersible at pH 7,  
20 C (P); pH7 as the CL salt; effective concentrations based on 100% active ingredients and mean  
measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;  
high concern for toxicity

significant mitigation of toxicity expected in the presence of 10 mg TOC/L, but has not been measured  
for this subclass of fatty polyamine;

assessment factor = 10.0

concern concentration = 0.010 mg/L (ppm)

## **PART V: RAD RISK RATIONALE: HUMAN HEALTH**

## **PART VI: SUMMARY OF EXPOSURE/RELEASE**

Proc/Use:

Releases via Incineration:

OR Landfill

Releases to Water:

OR Incineration OR Landfill

Fate: Releases to Water

SWC: 264.18 ppb

DW: LADD: 6.64E-06 mg/kg/d, ADD: 3.40E-04 mg/kg/d, ADR: 1.29E-02 mg/kg/d

Fish: LADD: 9.79E-07 mg/kg/d, ADD: 1.17E-02 mg/kg/d, ADR: 3.20E-03 mg/kg/d

>COC (10 ppb): 6 of 6 d/yr

## **PART VII: FOCUS DECISION AND RATIONALE**

**DISPOSITION:** Drop with non 5(e) SNUR

**RATIONALE:** P07-0563-0564 was dropped with a non 5(e) SNUR based on Eco concerns. The restriction in the SNUR will be the kg/yr production volume as specified in the PMN and no releases to water. Potential risks to human health were addressed by adequate dermal protection and negligible inhalation exposures. Although concerns were high, potential risks to the environment were low based on no significant exceedence of the 10 ppb COC. Recommended Eco testing will be the base set along with mitigation testing of suspended and dissolved carbon. No Fate testing was recommended.

## **PART VIII: CCD DISPOSITION / DD**

CCD:

## STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

Case #: P-07-0563-564

DCN:

SAT Date: 7/31/2007

SAT Chair:

L. Keifer

Submitter:

Cognis Oleochemicals LLC

Chemical Name:

CAS RN:

Structure

Molecular Formula:

Molecular Wt.

WT%&lt;500:

WT%&lt;1000:

MP:

BP:

&gt;500

Eq. Wt:

H2O Sol (g/L):

Dispersible

V.P.

&lt;0.000001

Max. Prod. Volume (kg/yr):

Physical State:

Solid

USE:

Emulsifier for oil mud drilling fluids

Consolidated set P-07-0563-64.

No references were found. Analog is an emulsifier for drilling fluid Amine

Related Case Numbers

Case Role

Related Case Numbers

Focus

Date: 8-8-07

Results:

Non 5 (2) SNUR



## STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

Case #: P-07-0564

DCN:

SAT Date: 7/31/2007

SAT Chair: L. Keifer

Submitter: Cognis Oleochemicals LLC

Chemical Name:

CAS RN:

## Structure

Molecular Formula:

Molecular Wt.

WT%&lt;500:

%&lt;1000:

MP:

BP:

&gt;500

Eq. Wt:

H2O Sol (g/L):

Dispersible

V.P.

&lt;0.000001

Max. Prod. Volume (kg/yr):

Physical State:

Solid

USE:

Emulsifier for oil mud drilling fluids

Consolidated set P-07-0563-64.

No references were found. Analog is an emulsifier for drilling fluid. Amine FGEW

Related Case Numbers

Case Role

Related Case Numbers

Focus

Date: 8-6-07

Results: Non 5 (ed) SMLR

STRUCTURE ACTIVITY TEAM REPORT

07/31/07

CASE NUMBER: P07-0563/0564

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:

HEALTH

ECOTOX

LEVEL OF CONCERN:

1-2

3

KEYWORDS: LUNG IRR-E,S,MM  
AQUATOX

SUMMARY OF ASSESSMENT

FATE: Estimations for low weight, [REDACTED]

Solid

log Kow = 2.90(E);

S = Disp./1.64 mg/L at 25 C (ICB/E)

VP < 1.0E-6 torr at 25 C (E)

BP > 400 C (E)

H < 1.00E-8 (E)

log Koc = 7.63(E)

log Fish BCF = 1.54(E)

POTW removal (%) = 50-90 via sorption and possible partial biodeg

Time for complete ultimate aerobic biodeg = mo

Sorption to soils/sediments = strong

PBT Potential: P1B1T1

\*CEB FATE: Migration to ground water = negl

HEALTH: Not absorbed from the skin as the neat material, poor absorption from the skin if in solution (pchem), poor absorption from the GI tract and moderate absorption from the lung (analog). Concern for surfactant effects on the lung; irritation to eye, skin (chronic), mucous membranes and lung based on surfactant properties of the compounds. Also concern for possible lung toxicity from cationic binding to lung membranes.

\*CEB HEALTH: Low moderate concern (Dermal, inhalation)

Test data: rat oral LD<sub>0</sub> = 2000 mg/kg

**Question for the economists:** Is [REDACTED] a reasonable production volume for the reported use as an emulsifier in oil drilling mud?

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50

<

1.0

P pH7 TOC<2

Predictions are based on SAR-nearest analog analysis for

[REDACTED] solid with mp unknown (P); S = dispersible at pH 7, 20 C (P); pH7 as the CL salt; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO<sub>3</sub>; and TOC <2.0 mg/L;

significant mitigation of toxicity expected in the presence of 10 mg TOC/L, but has not been measured for this subclass of fatty polyamine;

concern concentration = 0.010 mg/L (ppm)

SAT Co-chair: Leonard Keifer 564-8916

# GTOX Report

PMN No.  
**P-07-0563**

CAS No.

Rcvd:  
**07/23/07**

OECD  
Incomplet

ID: Rec# :

FA Name of Analog

Reviewer  
ked

|   | with activation               | without activation       | Positive Strains |
|---|-------------------------------|--------------------------|------------------|
| <u>Salmonella Assay:</u>                          | <input type="checkbox"/>      | <input type="checkbox"/> |                  |
| <u>Chromosomal Aberration</u>                     | CHO: <input type="checkbox"/> | <input type="checkbox"/> |                  |
|   | CHL: <input type="checkbox"/> | <input type="checkbox"/> |                  |
|   | V79: <input type="checkbox"/> | <input type="checkbox"/> |                  |
| <u>E. coli Reverse Mutation:</u>                  | <input type="checkbox"/>      | <input type="checkbox"/> |                  |
| <u>Mouse Micronucleus Assay:</u>                  | Route: <input type="text"/>   | <input type="checkbox"/> |                  |
| <u>Rat Hepatocytes Unscheduled DNA Synthesis:</u> |                               | <input type="checkbox"/> |                  |

## Other GTOX Results

## Comments

ECOTOX:

☒

Fate:

Aerobic degradability in seawater: Attachment 6

WS/Log P:

# Toxicology Report

PMN No.  
**P-07-0563**

CAS No.

Rcvd:  
**7/23/2007**

OECD  
**Incomplete**

ID: Rec#

S/A  
**S**

Name of Analog

Reviewer  
**ked**

Study#:  
**20**

Study Type

**ATOX**

Species

**RATS**

Sex

**MF**

Route

**GAVG**

## Test Substance Description

**Brown solid. Vehicle: Sesame oil.**

## Test Conditions

Study duration: 14 days; Strain: Wistar; Wt/Life stage: 148-150 g (F) and 170-190 g (M)/NS; No. Groups/No. Per Group: 1/10 (5 M and 5 F); Dose Level: 2000 mg/kg-bw; Test Conditions (Dose regimen): OECD TG 420. The study was initiated with a sighting study in which one female rat was given 2000 mg/kg bw of the test substance. Based on the results of the sighting study, the same procedure was carried out on five male and five female rats. A 14-day observation period followed dosing. All rats were killed on day 14 and subjected to gross necropsy.

## Results

The animal involved in the sighting study survived the treatment and showed slight signs of toxicity, including pinched abdomen and piloerection after 1, 3 and 6 hours of dosing. No abnormalities were observed at necropsy. All animals in the main study survived and showed marked signs of toxicity, including pinched abdomen and piloerection after 1 and 6 hours of dosing. No signs of pathological abnormalities were observed during gross necropsy. The oral LD50 was found to be above 2000 mg/kg bw.

## NCSAB SAT REPORT

PMN: P-07-0563

CAS RN:

Chemical Name:

Analog:

Production Volume:

Structure:

Use:

Emulsifier for oil mud drilling fluids.

Consolidated set P-07-0563-64.

No references were found. Analog is an emulsifier for drilling fluid. Amine FGEW =

Formula:

Eq Wt:

Mol Weight:

Wt% &lt; 500:

Wt% &lt; 1000

MP:

BP:

&gt; 500

VP:

&lt; 0.000001

H<sub>2</sub>O Sol (g/L):

Dispersible

Physical State:

Solid

Log P:

Endpoint (mg/L)

Est. Value

Meas. Value

Comments

Fish 96-h

&lt; 1

Daphnid 48-h

&lt; 1

Algal 96-h

&lt; 1

Fish ChV

&lt; 0.100

Daphnid ChV

&lt; 0.100

Algal ChV

&lt; 0.300

BCF

CHEMICAL CLASS:

SAR:

ECOTOX CONCERN

H

M

L

CONCERN CONCENTRATION

0.010

DATE

7/31/07

ASSESSOR:

## NCSAB SAT REPORT

PMN: P-07-0564

CAS RN:

Chemical Name:

Analog:

Production Volume:

Structure:

Use:

Emulsifier for oil mud drilling fluids.

Consolidated set P-07-0563-64.

No references were found. Analog is an emulsifier for drilling fluid. Amine FGEW =

Formula:

Eq Wt:

Mol Weight:

Wt% &lt; 500:

Wt% &lt; 1000

MP:

BP:

&gt; 500

VP:

&lt; 0.000001

H<sub>2</sub>O Sol (g/L):

Dispersible

Physical State:

Solid

Log P:

Endpoint (mg/L)

Est. Value

Meas. Value

Comments

Fish 96-h

&lt; 1.0

Daphnid 48-h

&lt; 1.0

Algal 96-h

&lt; 1.0

Fish ChV

&lt; 0.10

Daphnid ChV

&lt; 0.10

Algal ChV

&lt; 0.10

BCF

CHEMICAL CLASS:

SAR:

ECOTOX CONCERN

(H)

M

L

CONCERN CONCENTRATION

0.010

DATE

ASSESSOR: